

AD-A144 876

A PERTURBATION SOLUTION FOR RIGID DUMBEELL SUSPENSIONS. 1/1
IN STEADY SHEAR FLOW(U) WISCONSIN UNIV-MADISON
MATHEMATICS RESEARCH CENTER S KIM ET AL. JUN 84

UNCLASSIFIED

MRC-TSR-2700 DAAG29-80-C-0041

F/G 12/1

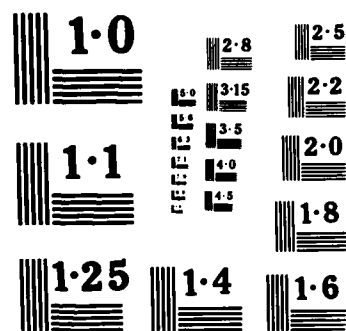
NL



END

FORMED

ONE



2

MRC Technical Summary Report #2700

A PERTURBATION SOLUTION FOR RIGID
DUMBBELL SUSPENSIONS IN STEADY
SHEAR FLOW

Sangtae Kim and Xijun Fan

AD-A144 876

**Mathematics Research Center
University of Wisconsin—Madison
610 Walnut Street
Madison, Wisconsin 53705**

June 1984

(Received January 4, 1984)

Approved for public release
Distribution unlimited

DTIC
ELECTE
S **D**
AUG 29 1984
E

Sponsored by

U. S. Army Research Office
P. O. Box 12211
Research Triangle Park
North Carolina 27709

National Science Foundation
Washington, D. C. 20550

84 08 24 04Z

DTIC FILE COPY

UNIVERSITY OF WISCONSIN-MADISON
MATHEMATICS RESEARCH CENTER

A PERTURBATION SOLUTION FOR RIGID DUMBBELL
SUSPENSIONS IN STEADY SHEAR FLOW

Sangtae Kim^{*,1} and Xijun Fan^{**,2}

Technical Summary Report #2700
June 1984

ABSTRACT

The orientation distribution function of a dumbbell undergoing rotary Brownian motion (with time constant λ) in steady shear flow, and the viscosity and normal stress coefficients are computed by a perturbation expansion in small, dimensionless shear rates $\lambda\dot{\gamma}$. It is found that the series expansions for both the viscosity and the first normal stress coefficient have identical radii of convergence at $\lambda\dot{\gamma} = 0.81$. By using analytical continuation, the solution was extended to $\lambda\dot{\gamma} = 1.5$, and checked with established results. Our results agree with earlier perturbation calculations of Kirkwood and Plock (1956), Bird and Warner (1971) and numerical calculations of Stewart and Sorenson (1972).

AMS (MOS) Subject Classifications: 76A05, 35L65

Key Words: rigid dumbbells, rotary Brownian diffusion, suspension

Work Unit Number 2 (Physical Mathematics)

*Department of Chemical Engineering, University of Wisconsin-Madison, Madison, WI 53706.

**Department of Mechanics, Zhejiang University, Hangzhou, Zhejiang, CHINA.

¹Sponsored by the United States Army under Contract No. DAAG29-80-C-0041, and the Du Pont Corporation.

²Supported by the National Science Foundation under Grant No. CPE-8104705.

SIGNIFICANCE AND EXPLANATION

Polymeric solutions play a central role in the manufacture of many plastics and especially, artificial fibres. A large research effort over decades has therefore been directed towards the prediction of the mechanical properties of such solutions which are important in manufacture, in particular, their viscosity and their normal stress.

It has turned out that many features found in a plot of the viscosity and normal stress coefficients vs. shear rate for polymeric solutions can be modeled qualitatively by a suspension of rigid dumbbells. Thus this model has been quite popular. Despite many attempts, exact analytical solutions have never been found for this problem although numerical and asymptotic results are available.

The following investigation establishes that the asymptotic solution for weak flows (or strong Brownian diffusion) is accurate only for dimensionless shear rates $\lambda\dot{\gamma}$ less than 0.81 where $\dot{\gamma}$ is the shear rate and λ is a material time constant for the rigid dumbbell model.

Accession For	
NTIS GRA&I	<input checked="" type="checkbox"/>
DTIC TAB	<input type="checkbox"/>
Unannounced	<input type="checkbox"/>
Justification	
By _____	
Distribution/	
Availability Codes	
Dist	Avail and/or Special
A-1	



The responsibility for the wording and views expressed in this descriptive summary lies with MRC, and not with the authors of this report.

A PERTURBATION SOLUTION FOR RIGID DUMBBELL SUSPENSIONS IN STEADY SHEAR FLOW

Sangtae Kim^{*,1} and Xijun Fan^{**,2}

INTRODUCTION

The rigid dumbbell in a Newtonian solvent under hydrodynamic and Brownian forces is a simple model of solutions of rigid macromolecules with both theoretical and pedagogical applications.^{1,2} In this note, we show that expansion solutions in small, dimensionless shear rates, $(\lambda\dot{\gamma})$, have a finite radius of convergence. We also show that these solutions can be analytically continued to a much larger domain by standard techniques for accelerating the convergence of series.

STATEMENT OF THE PROBLEM

Consider a dilute suspension (number of particles per unit volume, $n \ll 1$) of rigid axisymmetric particles, where hydrodynamic interaction is negligible between particles. The material functions can be determined from the orientation distribution function, $\psi(\theta, \phi)$, where $\psi(\theta, \phi) d\theta d\phi$ gives the fraction of particles with the axis oriented between $(\theta, \theta + d\theta)$ and $(\phi, \phi + d\phi)$. θ and ϕ are the usual spherical azimuthal and longitudinal angles. The equation of continuity and the equations of motion combine to give the "diffusion equation" for ψ , which for steady shear flow becomes²

$$\hat{\Lambda}\left(\frac{\psi}{\sin\theta}\right) - 6\lambda\dot{\gamma}\hat{\Omega}\left(\frac{\psi}{\sin\theta}\right) = 0. \quad (1)$$

with the operators $\hat{\Lambda}$, and $\hat{\Omega}$ defined as

* Department of Chemical Engineering, University of Wisconsin-Madison, Madison, WI 53706.

** Department of Mechanics, Zhejiang University, Hangzhou, Zhejiang, CHINA.

¹ Sponsored by the United States Army under Contract No. DAAG29-80-C-0041, and the Du Pont Corporation.

² Supported by the National Science Foundation under Grant No. CPE-8104705.

$$\hat{\Lambda}\psi = \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial\psi}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2\psi}{\partial\phi^2}$$

$$\hat{\Omega}\psi = \frac{\sin\phi \cos\phi}{\sin\theta} \frac{\partial}{\partial\theta} (\sin^2\theta \cos\theta \psi) - \frac{\partial}{\partial\phi} (\sin^2\phi \psi) .$$

We have defined our coordinate system such that $\frac{\partial v_x}{\partial y} = \dot{\gamma}$ is the only non-vanishing element of the velocity gradient tensor $\underline{\nabla v}$. For rigid dumbbells of length L , and bead friction coefficient ζ , the rotational time constant is given by $\lambda = \zeta L^2 / (12kT)$. The expression for λ for other axisymmetric shapes is given by Brenner.³

A general analytic solution of (1) has never been found although exact solutions of related equations such as Boeder's equation are known.⁴ Our objective is to solve equation (1) for ψ using a perturbation series in $\lambda\dot{\gamma}$ and to use the results to calculate the viscosity η and the first normal-stress coefficient ψ_1 (ψ_2 vanishes for this rigid dumbbell model):

$$\eta - \eta_s = \frac{1}{2} nkT\lambda \langle 2(P_0^0 - P_2^0) - P_2^2 \cos 2\phi \rangle_\psi \quad (2)$$

$$\psi_1 = \frac{nkT\lambda}{\dot{\gamma}} \langle P_2^2 \sin 2\phi \rangle_\psi \quad (3)$$

THE PERTURBATION SOLUTION

We expand ψ in powers of $\lambda\dot{\gamma}$

$$\psi(\theta, \phi) = \frac{1}{4\pi} \sum_{k=0}^{\infty} (6\lambda\dot{\gamma})^k \phi_k(\theta, \phi) \quad (4)$$

and substitute into the diffusion equation (1) to get the following hierarchy of equations for the ϕ_k :

$$\frac{n-\eta_s}{nkT\lambda} = \sum_{k=0}^{\infty} \left[A(1,1,2k) - \frac{1}{5} A(1,2,2k) - \frac{6}{5} A(2,2,2k) \right] (6\lambda\gamma)^{2k} \quad (8)$$

$$= \sum_{k=0}^{\infty} (-1)^k a_k (\lambda\gamma)^{2k}$$

$$\frac{5\psi_1}{6nkT\lambda^2} = \sum_{k=0}^{\infty} 12A(2,2,2k+1) (6\lambda\gamma)^{2k} \quad (9)$$

$$= \sum_{k=0}^{\infty} (-1)^k b_k (\lambda\gamma)^{2k}$$

The first twenty coefficients, a_k and b_k , are given in Table 1. The values for a_0 , a_1 and a_2 agree with Kirkwood and Plock⁵ and Bird and Warner.⁶

DISCUSSION

We note that the ratios a_{k+1}/a_k and b_{k+1}/b_k approach an asymptotic value with large k , i.e. approximately 1.521006. This result was tested by generating a_k and b_k up to $k = 85$, and it was found to hold for these higher coefficients as well. Therefore, the coefficients approach asymptotically to the coefficients of a geometric series in $(\lambda\gamma)^2$ with a radius of convergence of $(1.521006)^{-1/2} \doteq 0.81$. Therefore, our series solution converges only for $\lambda\gamma < 0.81$. However, since the coefficients approach those of a geometric series, we tried analytical continuation.

First, we replace the higher coefficients a_k and b_k for $k > N+1$ with their asymptotic counterparts \bar{a}_k and \bar{b}_k :

Table 1
Coefficients for the Series Solutions

k	a_k	b_k
0	1	1
1	0.5142 8571	1.0857 143
2	0.6888 3117	1.5475 724
3	1.0173 986	2.3156 606
4	1.5354 447	3.5063 866
5	2.3303 602	5.3265 547
6	0.3542 3678 $\times 10^1$	0.8098 9823 $\times 10^1$
7	0.5387 1583 $\times 10^1$	0.1231 7694 $\times 10^2$
8	0.8193 7480 $\times 10^1$	0.1873 5352 $\times 10^2$
9	0.1246 2985 $\times 10^2$	0.2849 7327 $\times 10^2$
10	0.1895 6859 $\times 10^2$	0.4334 6025 $\times 10^2$
11	0.2883 4481 $\times 10^2$	0.6593 1852 $\times 10^2$
12	0.4385 8958 $\times 10^2$	0.1002 8628 $\times 10^3$
13	0.6671 2099 $\times 10^2$	0.1525 4144 $\times 10^3$
14	0.1014 7310 $\times 10^3$	0.2320 2467 $\times 10^3$
15	0.1543 4667 $\times 10^3$	0.3529 2344 $\times 10^3$
16	0.2347 7055 $\times 10^3$	0.5368 1773 $\times 10^3$
17	0.3571 0009 $\times 10^3$	0.8165 3198 $\times 10^3$
18	0.5431 7067 $\times 10^3$	0.1241 9941 $\times 10^4$
19	0.8261 9517 $\times 10^3$	0.1889 1476 $\times 10^4$
20	0.1256 6924 $\times 10^4$	0.2873 5068 $\times 10^4$

$$\phi_1 = \frac{1}{12} p_2^2 \sin 2\phi \quad (5)$$

$$\hat{\Lambda}\phi_k = \hat{\Omega}\phi_{k-1} \quad k = 2, 3, 4 \dots$$

As pointed out by Kirkwood and Plock⁵ and by Bird and Warner⁶ the ϕ_k may be expressed as a linear combination of the spherical harmonics, due to the fact that

$$\hat{\Lambda}(P_n^m \begin{Bmatrix} \sin m\phi \\ \cos m\phi \end{Bmatrix}) = -n(n+1) P_n^m \begin{Bmatrix} \sin m\phi \\ \cos m\phi \end{Bmatrix} \quad (6)$$

$$\hat{\Omega}(P_n^m \begin{Bmatrix} \sin m\phi \\ \cos m\phi \end{Bmatrix}) = \sum_{j=m-2}^{m+2} \sum_{k=n-2}^{n+2} a_{nk}^{mj} p_k^j \begin{Bmatrix} \cos m\phi \\ -\sin m\phi \end{Bmatrix} \quad (7)$$

The a_{nk}^{mj} are tabulated in Table 1 of reference (6) and Table 11.4-1 of reference (2). Furthermore, from (7) it follows that $\cos m\phi$ terms appear only in the ϕ_k with k even, while $\sin m\phi$ terms appear only with k odd. Therefore, the material functions given by equations (2) and (3) reduce to a power series in $(\lambda\dot{\gamma})^2$ because of the orthogonality with respect to the ϕ integration. The perturbation results up to ϕ_4 are given in reference (2).

We have programmed this procedure (i.e. equations 4, 6 and 7), by generating a recursion formula for $A(m,n,k)$, where the m,n,k element is the coefficient of $P_{2(n-1)}^{2(m-1)}$ for ϕ_k . The coefficients generated by the program for ϕ_1 , ϕ_2 and ϕ_3 matched those given in reference (2). Because of orthogonality, only a few terms make a contribution to the material functions, i.e.:

$$\frac{\eta - \eta_s}{nkT\lambda} = \sum_{k=0}^N (-1)^k a_k (\lambda\tau)^{2k} + \sum_{k=N+1}^{\infty} (-1)^k \bar{a}_k (\lambda\tau)^{2k} \quad (10)$$

$$\frac{5\psi_1}{6nkT\lambda^2} = \sum_{k=0}^{\infty} (-1)^k b_k (\lambda\tau)^{2k} + \sum_{k=N+1}^{\infty} (-1)^k \bar{b}_k (\lambda\tau)^{2k} \quad (11)$$

with $\bar{a}_k = c_1 p^{-2k-2}$, $c_1 = 0.1879\dots$

$$p = 0.8108\dots$$

$\bar{b}_k = c_2 p^{-2k-2}$, $c_2 = 0.3582\dots$

$$p = 0.8108\dots$$

In the key step, the series is replaced by the equivalent continuation functions so that

$$\frac{\eta - \eta_s}{nkT\lambda} = \sum_{k=0}^N (-1)^k [a_k - \bar{a}_k] (\lambda\tau)^{2k} + c_1 [p^2 + (\lambda\tau)^2]^{-1} \quad (12)$$

$$\frac{5\psi_1}{6nkT\lambda^2} = \sum_{k=0}^N (-1)^k [b_k - \bar{b}_k] (\lambda\tau)^{2k} + c_2 [p^2 + (\lambda\tau)^2]^{-1} \quad (13)$$

By comparing with the exact numerical (collocation) solutions of Stewart and Sørensen⁷ we found that $N = 10$ was the optimum value. However, $N = 8, 9, 11$, and 12 also gave results which were accurate to four significant figures for $\lambda\tau < 1$. Table 2 shows the comparison between their collocation solution and

Table 2

Comparison of Stress Functions

$\lambda\dot{\gamma}$	$(n-n_s)/nkT\lambda$		$\psi_1/nkT\lambda^2$	
	<u>equation (12)</u> <u>N = 10</u>	<u>exact</u> <u>solution^a</u>	<u>equation (13)</u> <u>N = 10</u>	<u>exact</u> <u>solution^a</u>
0	1	1	6/5	6/5
0.1	0.9949	0.9949	1.1872	1.1872
0.125	0.9921	0.9921	1.1801	1.1801
0.25	0.9703	0.9703	1.1252	1.1252
0.3333	0.9502	0.9502	1.0749	1.0749
0.5	0.9029	0.9029	0.9588	0.9588
0.75	0.8306	0.8306	0.7874	0.7874
1.0	0.7676	0.7676	0.6467	0.6467
1.5	0.6604	0.6735	0.4596	0.4565
2.0833	-9.2	0.5998	-5.5	0.3289

^aCollocation calculations of Stewart and Sørensen.⁷

our extended solution (with $N = 10$, $c_1 = 0.18799972$, $c_2 = 0.35822745$,
and $p = 0.81082443$).

ACKNOWLEDGEMENTS: The authors thank Professor R. B. Bird for bringing our
attention to this problem and Professor W. E. Stewart and Dr. J. P. Sørensen
for furnishing details of their numerical calculations.

REFERENCES

- (1) W. Kuhn, Kolloid. Z., 68, 2-15 (1934).
- (2) R. B. Bird, O. Hassager, R. C. Armstrong, and C. F. Curtiss, Dynamics of Polymeric Liquids: Volume 2. Wiley, New York (1977).
- (3) H. Brenner, Int. J. of Multiphase Flow, 1, 195 (1974).
- (4) H. Brenner, J. Coll. Int. Sci., 34, 103 (1970).
- (5) J. G. Kirkwood and R. J. Plock, J. Chem. Phys., 24, 665 (1956).
- (6) R. B. Bird and H. R. Warner, Jr., Trans. Soc. Rheol., 15, 741 (1971).
- (7) W. E. Stewart and J. P. Sørensen, Trans. Soc. Rheol., 16, 1 (1972).

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER 2700	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) A PERTURBATION SOLUTION FOR RIGID DUMBBELL SUSPENSIONS IN STEADY SHEAR FLOW		5. TYPE OF REPORT & PERIOD COVERED Summary Report - no specific reporting period
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) Sangtae Kim and Xijun Fan		8. CONTRACT OR GRANT NUMBER(s) DAAG29-80-C-0041 CPE-8104705
9. PERFORMING ORGANIZATION NAME AND ADDRESS Mathematics Research Center, University of 610 Walnut Street Wisconsin Madison, Wisconsin 53706		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS Work Unit Number 2 - Physical Mathematics
11. CONTROLLING OFFICE NAME AND ADDRESS See Item 18 below.		12. REPORT DATE June 1984
		13. NUMBER OF PAGES 9
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)		15. SECURITY CLASS. (of this report) UNCLASSIFIED
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE
16. DISTRIBUTION STATEMENT (of this Report) Approved for public release; distribution unlimited.		
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)		
18. SUPPLEMENTARY NOTES U. S. Army Research Office P. O. Box 12211 Research Triangle Park North Carolina 27709 National Science Foundation Washington, D. C. 20550		
19. KEY WORDS (Continue on reverse side if necessary and identify by block number) rigid dumbbells rotary Brownian diffusion suspension		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) The orientation distribution function of a dumbbell undergoing rotary Brownian motion (with time constant λ) in steady shear flow, and the viscosity and normal stress coefficients are computed by a perturbation expansion in small, dimensionless shear rates $\lambda\dot{\gamma}$. It is found that the series expansions for both the viscosity and the first normal stress		

20. ABSTRACT - cont'd.

coefficient have identical radii of convergence at $\lambda\dot{\gamma} \doteq 0.81$. By using analytical continuation, the solution was extended to $\lambda\dot{\gamma} = 1.5$, and checked with established results. Our results agree with earlier perturbation calculations of Kirkwood and Plock (1956), Bird and Warner (1971) and numerical calculations of Stewart and Sorenson (1972).